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Figure SI1. Optimized structures of the 4 entgegen and the 4 zusammen conformers of AO-R obtained by quantum chemical calculations.



Figure SI2. Cyclized conformation of AO-R obtained by quantum chemical calculations.

Table SI1. Relative energy levels in cm<sup>-1</sup> (reference is the ground state of E1) of the ground and excited states of the 8 conformers of AO-R.

0/19629.4
543.2/20308.8
670.8/21176.6
1186.6/21752.8
3048.6/23414.3
4252.4/23772.2
4885.3/24496.2
5714.4/25212.9